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1RQI

DOI 10.2210/pdb1rqI/pdb

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☒ 1RQI

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Title

Active Conformation of Farnesyl Pyrophosphate Synthase Bound to Isopentenyl Pyrophosphate and Dimethylallyl S-Thiolodiphosphate

Authors

Hosfield, D.J., Zhang, Y., Dougan, D.R., Brooun, A., Tari, L.W., Swanson, R.V., Finn, J.

Primary Citation

Hosfield, D.J., Zhang, Y., Dougan, D.R., Brooun, A., Tari, L.W., Swanson, R.V., Finn, J. Structural basis for bisphosphonate-mediated inhibition of isoprenoid biosynthesis *J.Biol.Chem.* v279 pp.8526-8529, 2004
[Abstract]

History

Deposition 2003-12-05 Release 2004-03-02

Experimental Method

Type X-RAY DIFFRACTION Data N/A

Parameters

Resolution[Å]	R-Value	R-Free	Space Group
2.42	0.206 (obs.)	0.259	P 4 ₁ 2 2

Unit Cell

Length [Å]	Angles [°]	a	b	c
88.84	90.00	88.84	90.00	174.77
90.00	90.00	90.00	90.00	90.00












Molecular Description Asymmetric Unit

Polymer: 1 Molecule: Geranyltranstransferase Chains: A,B EC no.: 2.5.1.10

Classification

Transferase



Source	Polymer: 1		Scientific Name: Escherichia coli			Common Name: Bacteria		Expression system: Esc	
Chemical Component	Identifier	Name		Formula		Drug Similarity	Hapten Similar		
SCOP Classification (version 1.71)	MG	MAGNESIUM ION		Mg ²⁺					
	IPR	ISOPENTYL PYROPHOSPHATE		C ₅ H ₁₄ O ₇ P ₂					
	DST	DIMETHYLLALLYL S-THIOLODIPHOSPHATE		C ₅ H ₁₄ O ₆ P ₂ S					
	DPO	DIPHOSPHATE		O ₇ P ₂ ⁴⁻					
SCOP Classification (version 1.71)	Domain Info	Class	Fold	Superfamily		Family	Domain		
CATH Classification (version v3.0.0)	d1rqia_	All alpha proteins	Terpenoid synthases	Terpenoid synthases		Isoprenyl diphosphate synthases	Farnesyl diphosphate synthase (geranyltrans		
	d1rqib_	All alpha proteins	Terpenoid synthases	Terpenoid synthases		Isoprenyl diphosphate synthases	Farnesyl diphosphate synthase (geranyltrans		
CATH Classification (version v3.0.0)	Domain	Class	Architecture		Topology				
PFAM Classification	1rqIA00	Mainly Alpha	Orthogonal Bundle		Farnesyl Diphosphate Synthase				
	1rqIB00	Mainly Alpha	Orthogonal Bundle		Farnesyl Diphosphate Synthase				
PFAM Classification	Chain	PFAM Accession	PFAM ID	Description		Type			
GO Terms	A	PF00348 	polyprenyl_synt	Polyprenyl synthetase		Domain			
	B	PF00348 	polyprenyl_synt	Polyprenyl synthetase		Domain			
GO Terms	Polymer	Molecular Function		Biological Process					
	Geranyltransferase (1RQI:A,B)	• none		• isoprenoid biosynthetic process		C			

WEST Search History

DATE: Friday, March 23, 2007

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		<i>DB=PGPB,USPT,USOC,EPAB,JPAB,DWPI; PLUR=YES; OP=ADJ</i>	
<input type="checkbox"/>	L7	L1 and (Brooun\$ or Dougan\$ or Hosfield\$ or Zhang\$).in.	10
<input type="checkbox"/>	L6	L1 and ispA	9
<input type="checkbox"/>	L5	L4 and ispA	2
<input type="checkbox"/>	L4	L3 and coordinate	61
<input type="checkbox"/>	L3	L2 and coli	164
<input type="checkbox"/>	L2	L1 and crystal structure	198
<input type="checkbox"/>	L1	farnesyl and synthase and crystal	501

END OF SEARCH HISTORY

STN

10651668

=> d his

(FILE 'HOME' ENTERED AT 14:50:27 ON 23 MAR 2007)

FILE 'CAPLUS' ENTERED AT 14:50:44 ON 23 MAR 2007

L1 57 S FARNESYL AND SYNTHASE AND CRYSTAL
L2 2 S L1 AND ISPA

=> d L2 1-2

L2 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2005:1178062 CAPLUS
DN 143:418026
TI Pseudomonas aeruginosa gene ispA farnesyl diphosphate
synthase, its cloning, and biochem. and biophys. characterization
useful for drug design
IN Edwards, Aled; Dharamsi, Akil; Vedadi, Masoud; Kimber, Matthew; Vallee,
Francois
PA Affinium Pharmaceuticals, Inc., Can.
SO U.S. Pat. Appl. Publ., 154 pp., Cont.-in-part of Appl. PCT/CA03/00714.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	US 2005245728	A1	20051103	US 2004-967671	20041018
	WO 2003097789	A2	20031127	WO 2003-CA714	20030521
	WO 2003097789	A3	20040205		
PRAI	US 2002-382443P	P	20020521		
	WO 2003-CA714	A2	20030521		

L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:931464 CAPLUS
DN 140:2343
TI Cloning and physical characterization of farnesyl diphosphate
synthase from Pseudomonas aeruginosa and its use as a
antimicrobial target
IN Edwards, Aled; Dharamsi, Akil; Vedadi, Masoud; Mansoury, Kamran; Houston,
Simon; Vallee, Francois; Kimber, Matthew
PA Affinium Pharmaceuticals, Inc., Can.
SO PCT Int. Appl., 240 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	---	-----	-----	-----
PI	WO 2003097789	A2	20031127	WO 2003-CA714	20030521
	WO 2003097789	A3	20040205		
	AU 2003229452	A1	20031202	AU 2003-229452	20030521
	US 2005245728	A1	20051103	US 2004-967671	20041018
PRAI	US 2002-382443P	P	20020521		
	WO 2003-CA714	W	20030521		

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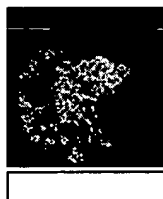
Help **34 Structure Hits** 8 Citations 28 Ligand Hits 2 Web Page Hits

1 2 3 4 ➔

☒ **1WCO**



THE SOLUTION STRUCTURE OF THE NISIN-LIPID II COMPLEX



Characteristics

Release Date: 07-Mar-2005 Exp. Method: NMR 20 Structu

Classification

Antibiotics

Compound

Polymer: 1 Molecule: ALA-DGL-LYS-DAL-DAL PEPT
Chains: L
Polymer: 2 Molecule: NISIN Chains: N Other
Details: THIOETHER BONDS (LANTHIONINE
LINKAGES) BETWEEN N3-N7, N8-N11, N13-N19, I
N26, N25-N28

Authors

Hsu, S.-T.D., Breukink, E., Tischenko, E., Lutter,
M.A.G., De Kruijff, B., Kaptein, R., Bonvin,
A.M.J.J., Van Nuland, N.A.J.

☒ **1ZW5**



**X-ray structure of Farnesyl diphosphate
synthase protein**

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